CHAPTER III
MATHEMATICAL MODELING

3.1 Model Structure of the Process

3.1.1 Gravitational Flow Tank

The structure of a gravitational flow tank is composed of tank and pipe line with water fed in and drained out of the tank. (Process Modeling, Simulation, and Control for Chemical Engineers, William L. Luyben)

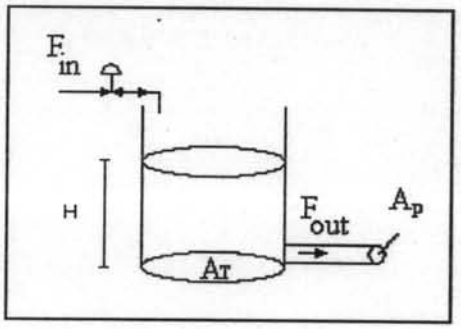

Figure 3.1 Gravitational flow tank.

Gravitational flow tank data are shown in Table 3.1

Table 3.1 Gravitational flow tank data

	Pipe:	Tank:	Unit
ID=	3	12	ft
Area=	7.06	113	ft^2
Length=	3000	-	ft
Height=	-	7	ft
Steady-state values:			
F=	35.1 ft^3/s(15,700 gpm)		
h=	4.72 ft		
v=	4.97 ft/s		
Parameters:			
Reynolds number=	1,380,000		
Friction factor=	0.0123		
KF=	$2.81*10^{-2}$ $lb_f/(ft/s)^2$ ft		

For the gravitational flow tank, it is without a reaction in the system. For the level control, a differential equation for the gravitational flow tank model is composed of force balance and total continuity equations, which are:

$$\frac{dv}{dt} = \frac{g}{L}h - \frac{K_F g_C}{\rho A_p}v^2 \qquad \text{for force balance} \qquad (3.1)$$

$$A_T \frac{dh}{dt} = F_{in} - F_{out} \qquad \text{for total continuity} \qquad (3.2)$$

where

H is the height of liquid level in tank (ft).

A_T is the area of tank =113 ft^2.

F_{in} is the liquid flow rate in (ft^3/s).

F_{out} is the liquid flow rate out (ft^3/s).

v is the velocity at outlet line (ft/s).

t is the time (second).

g is the gravitational acceleration = 32.2 ft/s^2.

ρ is the density of liquid = 62.47 lb/cu.ft.

L is the length of pipe (ft).

g_c is the conversion factor = 32.2 $lb_m*ft/(lb_f*s^2)$.

The new values of H and v at the $(n+1)^{th}$ step are calculated from the explicit Euler algorithm with a step size of DELTA. The equations are shown in equation 3.3 and 3.4:

$$(H)_{n+1} = (H)_n + DELTA(dH)_n \quad (3.3)$$

$$(v)_{n+1} = (v)_n + DELTA(dv)_n \quad (3.4)$$

where

DELTA is the 1 second.

n is the time index.

3.1.2 Plug-flow Reactor and Continuous Stirred Tank Reactor (CSTR)

A model of the plug-flow reactor and CSTR is shown in Figure 3.2. Chemical A is the reactant of the reaction.

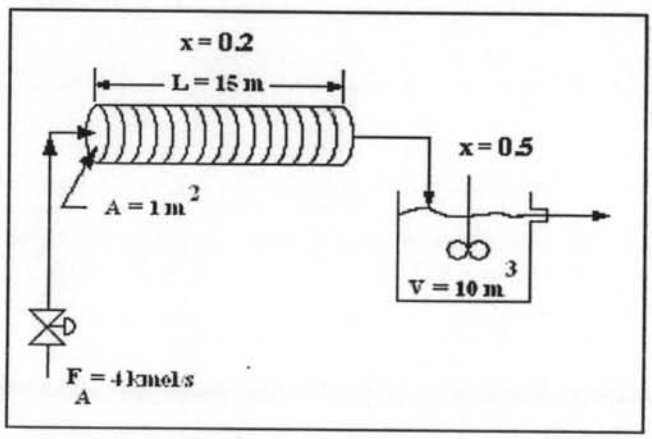

Figure 3.2 Plug-flow reactor and CSTR.

Initial concentration of reactant A, C_{A0}, is 20 kmol/m^3. Feed rate is 4 kmol/s. Output concentration at steady-state is 16.14 kmol/m^3. Dead time is 15 seconds. The conversion, x, is 0.2 and 0.5 for plug-flow and CSTR, respectively.

Differential equations in this system are composed of mole balances equation of plug-flow and CSTR, which are:

$$\frac{-dF_A}{dV} = -r_A \qquad \text{for plug-flow reactor} \qquad (3.5)$$

$$V = \frac{F_{0A} - F_A}{-r_A} \qquad \text{for CSTR} \qquad (3.6)$$

$$r_A = -\frac{dC_A}{dt} \qquad \text{for chemical reaction} \qquad (3.7)$$

where

F_{A0} is molar flow rate at initial of reactant A (kmol/s).

F_A is molar flow rate of reactant A (kmol/s).

V is volume of reactor of reactant A (m^3).

r_A is rate reaction of reactant A.

C_A is concentration of reactant A ($kmol/m^3$) = $C_{A0}(1-x)$.

C_{A0} is initial concentration of reactant A ($kmol/m^3$).

The new value of C_A at the $(n+1)^{th}$ step are calculated from the explicit Euler algorithm with a step size of DELTA. The equations are shown in equation 3.8:

$$(C)_{n+1} = (C)_n + \text{DELTA}(dC_A)_n \qquad (3.8)$$

where

DELTA is the 1 second.

n is the time index.

3.1.3 Binary Distillation Column

A dynamic model of a depropanizer column is developed in this thesis. The column is composed of a condenser and a reboiler, counted as two stages.

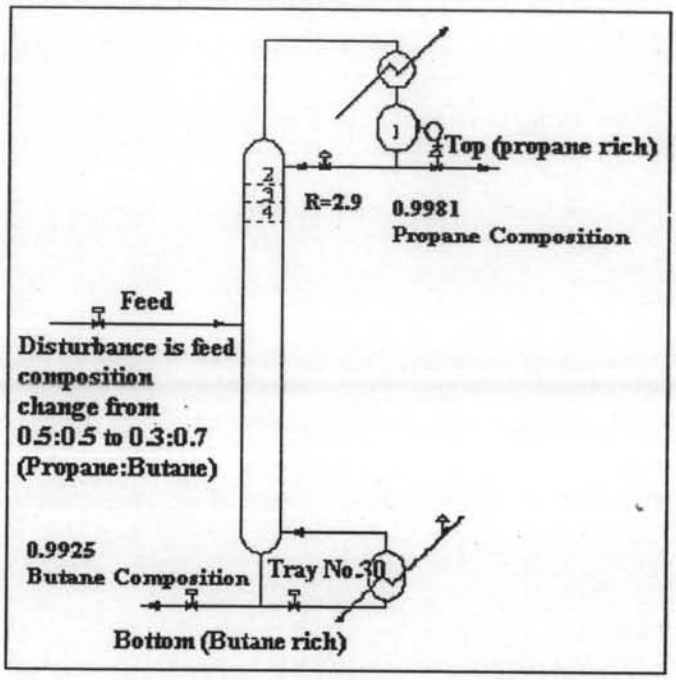

Figure 3.3 Conventional depropanizer column.

There are 30 stages for the column. The first stage is the total condenser and reflux drum and the last stage is the reboiler. The number of trays of the column, including reboiler and condenser, is 30. Reflux ratio, R, is 2.90. Feed flowrate is at 0.09 kg-mol/minute. The feed is a mixture of propane and butane at ratio 0.5:0.5 (propane:butane). The feed enters at tray no.15 with a pressure of 17 bars and a temperature of 369 K. The product specification of mole fraction is 0.9981 for propane at the top and 0.9925 for butane at the bottom. The pressure drop of the column is assumed constant at 0.065 bars. The pressure in reflux drum is equal to 16 bars.

For a dynamic simulation, changes in mass and energy are formulated as differential equations. There are material (equation 3.9), component (equation 3.9), and energy (equation 3.9) balances.

$$\frac{dM_n}{dt} = F + L_{n+1} + V_{n-1} - L_n - V_n \tag{3.9}$$

$$\frac{dx_i M_n}{dt} = z_{i,f} F + x_{i,n+1} L_{n+1} + y_{i,n-1} V_{n-1} - x_{i,n} L_n - y_{i,n} V_n \tag{3.10}$$

$$\frac{dh_n^L M_n}{dt} = h_F F + h_{n+1}^L L_{n+1} + h_{n-1}^V V_{n-1} - h_n^L L_n - h_n^V V_n \qquad (3.11)$$

where

L is the liquid molar flow rate (kmol/30 s).

V is the vapor molar flow rate (kmol/30 s).

F is the feed molar flow rate (kmol/30 s).

x is the molar fraction in liquid.

y is the molar fraction in vapor.

z is the molar fraction in feed.

h^l is the liquid molar enthalpy (kj/kmol).

h^v is the vapor molar enthalpy (kj/kmol).

h_F is the feed molar enthalpy (kj/kmol).

M is the tray liquid hold up (kmol).

n is the index number of tray =1, 2, …, 30.

i is the index number of component.

It is essential to have an accurate model or correlation for the vapor-liquid equilibrium (VLE) and the physical properties of the component in the distillation tower. There are many useful sources for obtaining literature data and correlating equations to represent the system. The phase equilibrium of some systems is essentially ideal (Practical Distillation Control, William L. Luyben), which are:

$$y_i P = x_i P_i^s \qquad \text{for Raoult's law} \qquad (3.12)$$

$$K_i = \frac{y_i}{x_i} \qquad \text{for equilibrium constant} \qquad (3.13)$$

where

y_i is the vapor composition (mole fraction).

x_i is the liquid composition (mole fraction).

P is the total pressure (bars).

P_i^s is the vapor pressure (bars).

K_i is the equilibrium constant.

Pure component vapor pressure is calculated by the Antoine equation, as shown in equation 3.14:

$$\ln(P_i^s) = C_1 + \frac{C_2}{C_3 + T} \tag{3.14}$$

where

C_1, C_2, and C_3 are the Antoine coefficients

Energy plays an important part in distillation. Liquid enthalpy is not a function of pressure because liquids are incompressible. Liquid and vapor enthalpy equations are formulated by using data from IFP-school (Institut Français de pétrole). It is valid in the range between 40°C and 130°C. The data of liquid and vapor enthalpy are shown in appendix D.

Liquid flow rate calculation is done by the Francis Weir Formula (Practical Distillation Control, William L. Luyben), which is:

$L_n = C\rho_n^L w_{len} H_{ow}^{1.5}$ for Francis Weir Formula (3.15)

Where

C is the constant for unit's conversion.

ρ^L_n is the density of liquid at n^{th} tray (1000 kg/m^3).

w_{len} is the weir length (m).

H_{ow} is the height of liquid above weir height (m).

The density of the liquid is an important value in the model. The Racckett equation (Chemical properties handbook, Carl L. Yaws) is used in the model for calculating the density of the liquid in the model:

$$\rho_i^L = A * B^{-\left(1-\frac{T}{T_C}\right)^n} \tag{3.16}$$

where

A, B, n are the regression coefficients.

T_C is the critical temperature of component i (K).

The model assumes that the single flow passes the hydraulics tray. The liquid enters the tray through the down comer of the above tray. Vapor enters the tray from the tray below. The vapor and liquid are completely mixed on the tray. Vapor leaves the tray, in equilibrium with the tray liquid composition, and passes to the above tray. The liquid flows over the outlet weir into the down comer and the tray below. The tray may contain a feed or a side stream. A dynamic model for the

tray will contain N_c differential equations of material balances, where N_c is the number of components in the system, and overall energy balance (Practical Distillation Control, William L. Luyben). Numerical methods to solve the equations are shown in appendix E.

3.2 Model of the Control System

3.2.1 Control System

The control system is used for controlling the process to get the output from system on specification. This thesis focuses on the proportional-integral derivative (PID) control system and dynamic matrix control.

3.2.1.1 PID Control

There are many types of control systems in the process. The conventional controller is the proportional-integral-derivative (PID) controller. This controller was used in many processes. A proportional controller gain (K_C) reduces the rise time and the steady-state error as K_C increases. It cannot eliminate error in the controlled variable. An integral control (τ_I) eliminates the steady-state error, but it may make the transient response become underdamped. A derivative control (τ_D) increases the stability of the system, reducing the overshoot, and improving the transient response. The signal sent to the manipulated variable is calculated from equation 3.17. The PID control system has feedback and feed forward controls. The block diagrams of feedback and feed forward control are shown in Figures 3.4 and 3.5:

$$\Delta Y = K_C e + \frac{1}{\tau_I}\int_0^{\infty} \int e dt + \tau_D \frac{de}{dt} + bias \qquad (3.17)$$

where

ΔY is the signal sent to manipulated variable.

e is the error= (setpoint-controlled variable).

K_C is the proportional gain.

τ_I is the integral time or reset time.

τ_D is the derivative time constant.

bias is the signal of manipulated variable with out error.

t is the time.

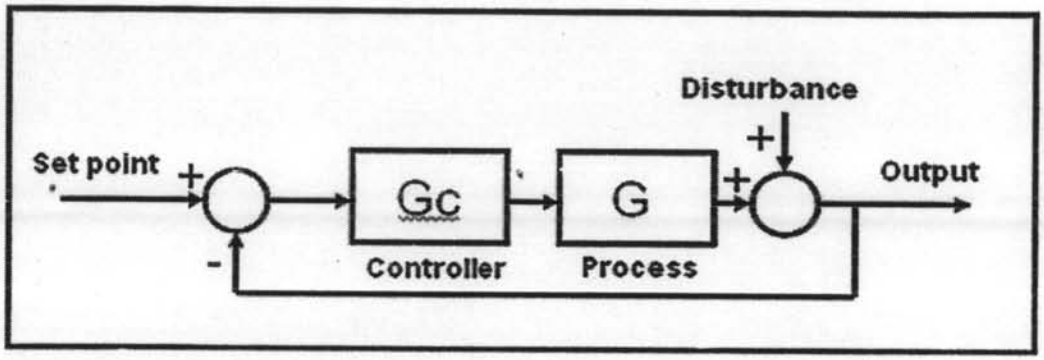

Figure 3.4 Block diagram of PID feedback control.

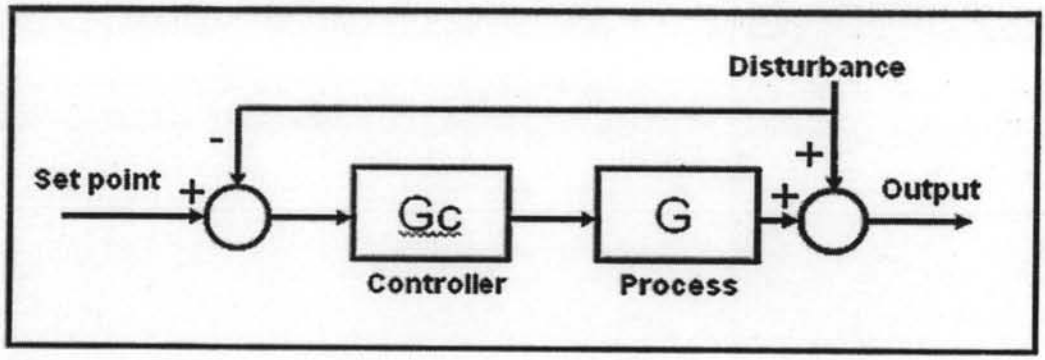

Figure 3.5 Block diagram of PID feedforward control.

3.2.1.2 Cascade Control

A cascade control structure has two controllers with the output of the primary (or master) controller changing the setpoint of the secondary (or slave). There are two purposes for cascade control: (1) to eliminate the effects of some disturbances, and (2) to improve the dynamic performance of the control loop (Process Modeling, Simulation, and Control for Chemical Engineers, William L. Luyben).

As shown in Figure 3.6, the primary controller is the feed back control (level control, LC) and the secondary controller is the feed forward control (FFC) or flow control. The block diagram of cascade control is shown in Figure 3.7.

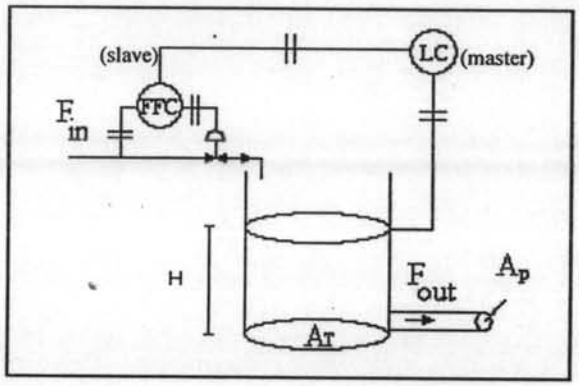

Figure 3.6 Gravitational flow tank with cascade control.

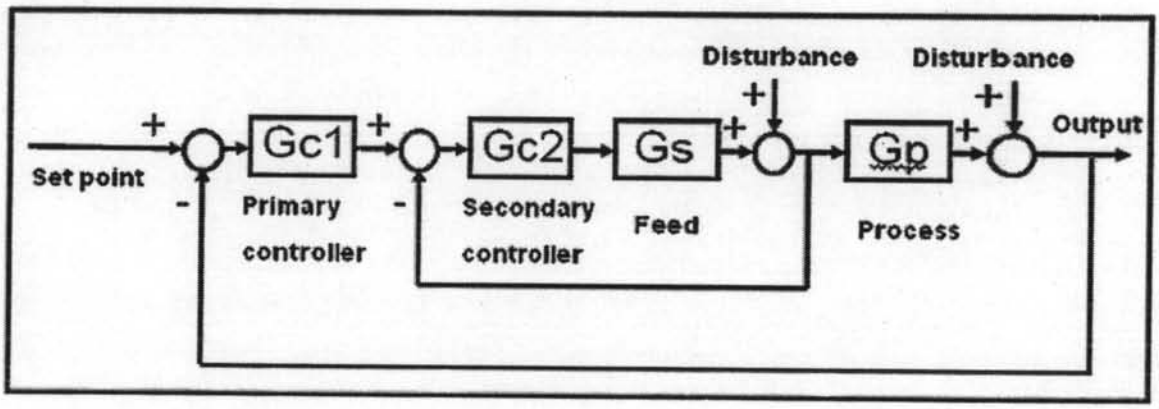

Figure 3.7 Block diagram of cascade control.

3.2.1.3 Dynamic Matrix Control

Advanced controllers, called dynamic matrix control (DMC), one of the model predictive controls, has become popular over the past two decades. This is a time-domain method that uses a model of the process to calculate future changes in the manipulated variable.

The DMC shown in Figure 3.8 is operated like the feedback control in that it measures the output and calculates the manipulated variable move.

The DMC will predict the controlled variable in the future before calculating the manipulated variable move. The block diagram of a DMC is shown in Figure 3.9.

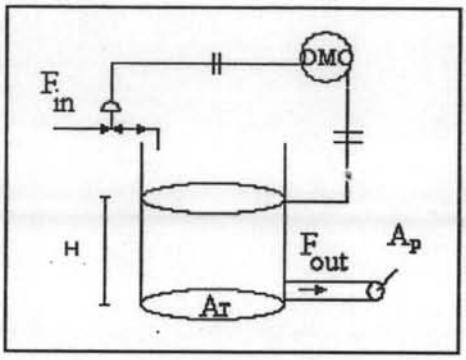

Figure 3.8 Gravitational flow tank with dynamic matrix control.

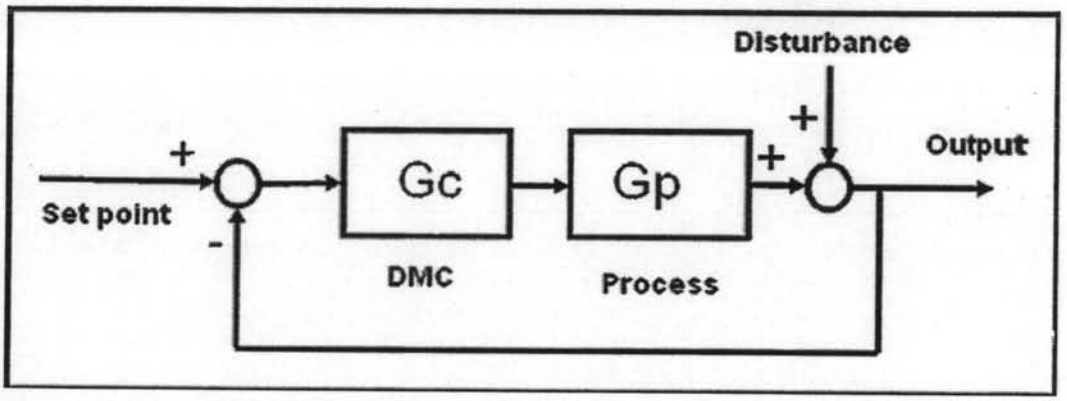

Figure 3.9 Block diagram of DMC.

The equation used to generate the DMC controller gain and manipulated variable movement is related to matrix form, B (equation 3.18). This matrix comes from the response curve of the control variable of the process model without controller by unit step change in manipulated variable as shown in Figure 3.10.

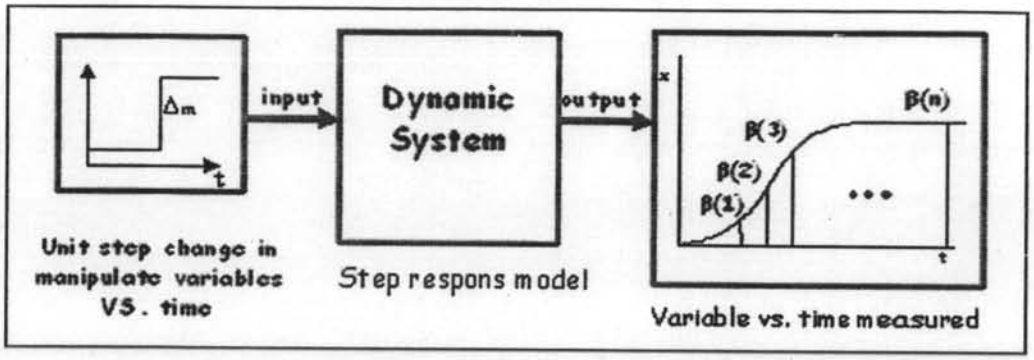

Figure 3.10 Unit step-response function.

Results are collected and rearranged to matrix form B.

$$B = \begin{bmatrix} \beta(1) & 0 & \dots & 0 \\ \beta(2) & \beta(1) & 0 & \dots \\ \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots \\ \beta(NP) & \beta(NP-1) & \dots & \beta(NP+1-NC) \end{bmatrix}_{NPXNC} \tag{3.18}$$

Correlating to Figure 3.10, the relationship between measured variable, x, and step change of manipulated variable, Δm, at all t, is shown in equation 3.19. The matrix, B, is used to generate the DMC controller gain by this equation:

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \dots \\ x_{NP} \end{bmatrix}_{NPX1} = \begin{bmatrix} \beta(1) & 0 & \dots & 0 \\ \beta(2) & \beta(1) & 0 & \dots \\ \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots \\ \beta(NP) & \beta(NP-1) & \dots & \beta(NP+1-NC) \end{bmatrix}_{NPXNC} \begin{bmatrix} \Delta m_1 \\ \Delta m_2 \\ \Delta m_3 \\ \dots \\ \Delta m_{NC} \end{bmatrix}_{NCX1} \tag{3.19}$$

where

NC is the number of the time interval of the manipulated variable moves in the future.

NP is the number of the time interval of the controlled variable change that covers 90 to 95 % of the system response.

Δm is the manipulated variable move.

x is the controlled variable.

Equation 3.19 can be rewritten to equation 3.20:

$$\Delta m = K_{DMC} E^f \tag{3.20}$$

$$K_{DMC} = \left(B^T B\right)^{-1} B^T \tag{3.21}$$

$$E^f = \left(SP_i - CV_i^f\right) \tag{3.22}$$

where

K_{DMC} is the matrix form of DMC controller gain.

B is the matrix of the unit step-response function.

E^f is the matrix error.

SP_i is the matrix set point.

CV^f_i is the matrix of predicted controlled variable at i^{th} sampling period. (measured variable)

Δm is the manipulated variable.

The DMC controller will predict the control variable in the future step time by equation 3.23:

$$CV_i^f = CV_{meas} + \sum_{k=0}^{-NP+1} \left[\beta_{i+1-k} - \beta_{1-k}\right]\left(\Delta m_k\right)^{old} \tag{3.23}$$

Where

$CV^f{}_i$ is the predicted value of control variable at i^{th} sampling period.

CV_{meas} is the measure controlled variable at present time.

β is the value of controlled variable from step response matrix, B.

Δm is the manipulated variable move.

NP is the number of the time interval of the controlled variable change that covers 90 to 95 % of the system response.

Controller gain, K_{DMC}, is multiplied by error to get manipulated variable movement, Δm, where the error is found from set point minus predicted value of control variable in the future.

The performance index will include magnitudes of the Δm values. Equation 3.20 and equation 3.21 will change to equation 3.24 and equation 3.25 to improve the performance of the controller gain with tuning parameter f,

which prevents large changes in the manipulated variable. (Process modeling, simulation, and control for chemical engineers, William L. Luyben)

$$\Delta m = K_{DMC} E^f \tag{3.24}$$

$$K_{DMC} = \left[B^T B + f^2 I\right]^{-1} B^T \tag{3.25}$$

where

f is the weighting factor .

I is the identity matrix.

The DMC algorithm has the following steps at each point in time:

1. Using step response to process model without controller and collecting measured variable to form matrix, B, in equation 3.18.
2. Using matrix, B, from step 1 to find K_{DMC} from equation 3.26.
3. Calculating CV^f_i from equation 3.23.
4. Calculating E^f from equation 3.22.
5. Calculating ΔMV from equation 3.24.
6. Changing manipulated variable by ΔMV_1.
7. At the next sampling period, measuring the controlled variable to get a new value of control variable and repeating the step 3 to 7.

Figure 3.11 shows the dynamic response of variables for the DMC control.

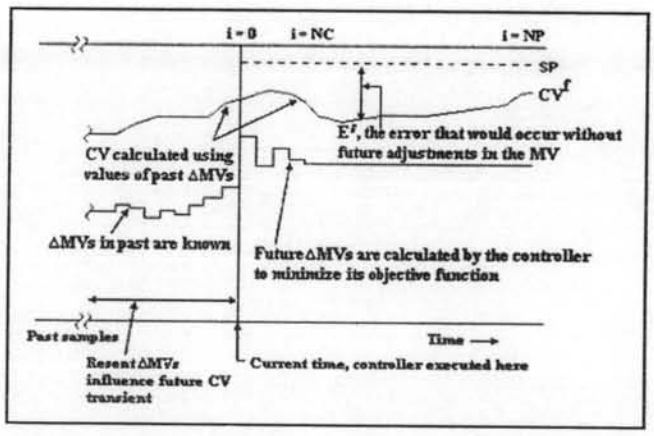

Figure 3.11 Dynamic response of variables for DMC control.

3.2.2 Controller Tuning

There are many controller tuning methods for PID controller. This work has used the basic controller tuning method which is the Ziegler-Nichols method. The steps of the tuning method are shownbelow. For DMC, a tuning method uses three parameters; NP, NC, and f.

3.2.2.1 Ziegler-Nichols: Closed Loop

This method was found by J. G. Ziegler and N. B. Nichols in 1942. They give reasonable first guesses of settings. Steps of tuning the PID control by Ziegler-Nichols are shown below.

Step 1 - Set controller to process with low gain, no reset, τ_I, or derivative, τ_D.

Step 2 - Gradually increase gain until oscillation occurs.

Step 3 - Record the gain at oscillation, called ultimate gain (Kcu), and time period, called ultimate period (Pu).

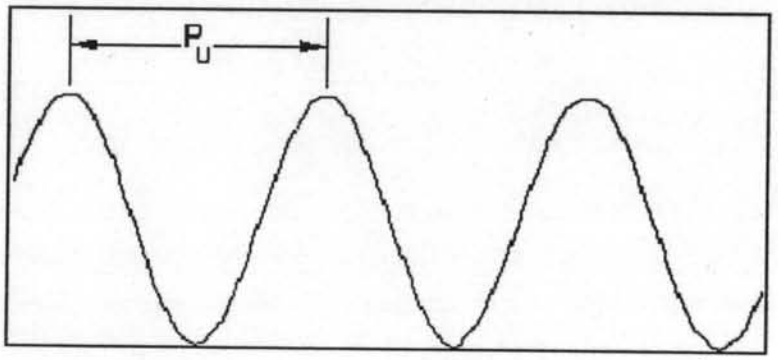

Figure 3.12 Oscillation with a constant amplitude.

The gain (K_C), reset (τ_I), and derivative (τ_D) are calculated using criteria in Table 3.2.

Table 3.2 Tuning parameters for Ziegler Nichols tuning method: closed loop (Process Dynamics, Modeling, and Control, William L. Luyben)

	Gain (K_C)	Reset (τ_I)	Derivative (τ_D)
P	$K_{CU}/2$	-	-
PI	$K_{CU}/2.2$	Pu/1.2	-
PID	$K_{CU}/1.7$	Pu/2	Pu/8

3.2.2.2 Tuning of Dynamic Matrix Control

The tuning parameters of this control system are NC, NP, and f. The definitions of NC, NP, and f are shown below:

- NC is the number of the time interval of the manipulated variable moves in the future. NC is typically set at 50 % of NP.
- NP is the number of the time interval of the controlled variable change that covers 90 to 95 % of the system response.
- f is weighting factor preventing large changes in manipulated variable.

Effect of f on control is that when f is small, it will cause high oscillation in the controlled variable. When f is large, the controlled variable will reach the set point slower. In this thesis, f is adjusted manually.